



(51) International Patent Classification:

G06F 19/10 (2011.01)

(21) International Application Number:

PCT/US2013/031661

(22) International Filing Date:

14 March 2013 (14.03.2013)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

61/652,076

25 May 2012 (25.05.2012)

US

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(81) Designated States (unless otherwise indicated, for every

kind of national protection available): AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY,

BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Declarations under Rule 4.17:

— of inventorship (Rule 4.17(iv))

Published:

— with international search report (Art. 21(3))

— with sequence listing part of description (Rule 5.2(a))

(54) Title: SYSTEM AND METHOD FOR PREDICTING THE IMMUNOGENICITY OF A PEPTIDE

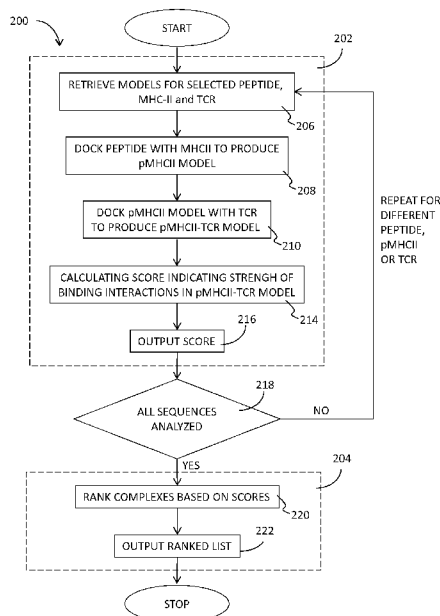


FIG. 2

(57) Abstract: A system, computer readable storage medium and method of predicting the immunogenicity of a peptide are provided. In certain cases the system includes: a) a model of a peptide, a model of a MHCII protein and a model of a T cell receptor; and b) an executable program for: (i) evaluating the strength of intermolecular interactions of a complex containing the peptide, the MHCII protein and the T cell receptor to provide a score that predicts the immunogenicity of the peptide; and (ii) outputting the score.